

Calculation of Predicted Hit and Predicted No-Hit Reliabilities

Dependence on Hit-NoHit Distributions

Fraction Hit (%Hit)	Fraction No-Hit (%No-Hit)	False Negative (FN)	False Positive (FP)	Predicted	Predicted	Overall Reliability (OR)
				Hit Reliability (PH)	No-Hit Reliability (PNH)	
0.1	0.9	0.2	0.2	0.308	0.973	0.800
0.2	0.8	0.2	0.2	0.500	0.941	0.800
0.3	0.7	0.2	0.2	0.632	0.903	0.800
0.4	0.6	0.2	0.2	0.727	0.857	0.800
0.5	0.5	0.2	0.2	0.800	0.800	0.800
0.6	0.4	0.2	0.2	0.857	0.727	0.800
0.7	0.3	0.2	0.2	0.903	0.632	0.800
0.8	0.2	0.2	0.2	0.941	0.500	0.800
0.9	0.1	0.2	0.2	0.973	0.308	0.800
0.1	0.9	0.2	0.35	0.203	0.967	0.665
0.2	0.8	0.2	0.35	0.364	0.929	0.680
0.22	0.78	0.2	0.35	0.392	0.920	0.683 Approx. high screen
0.3	0.7	0.2	0.35	0.495	0.883	0.695
0.4	0.6	0.2	0.35	0.604	0.830	0.710
0.5	0.5	0.2	0.35	0.696	0.765	0.725
0.6	0.4	0.2	0.35	0.774	0.684	0.740
0.7	0.3	0.2	0.35	0.842	0.582	0.755
0.8	0.2	0.2	0.35	0.901	0.448	0.770
0.9	0.1	0.2	0.35	0.954	0.265	0.785
0.1	0.9	0.1	0.1	0.500	0.988	0.900
0.2	0.8	0.1	0.1	0.692	0.973	0.900
0.3	0.7	0.1	0.1	0.794	0.955	0.900
0.4	0.6	0.1	0.1	0.857	0.931	0.900
0.5	0.5	0.1	0.1	0.900	0.900	0.900
0.6	0.4	0.1	0.1	0.931	0.857	0.900
0.7	0.3	0.1	0.1	0.955	0.794	0.900
0.8	0.2	0.1	0.1	0.973	0.692	0.900
0.9	0.1	0.1	0.1	0.988	0.500	0.900

Predicted Hit Reliability = correctly predicted hits / (correctly predicted hits + incorrectly predicted hits)

$$PH = (1 - FN)(%H) / [(1 - FN)(%H) + FP(%NH)]$$

Predicted No-Hit Reliability = correctly predicted no-hits / (correctly predicted no-hits + incorrectly predicted no-hits)

$$PNH = (1 - FP)(%NH) / [(1 - FP)(%NH) + FN(%H)]$$

Overall Reliability = (correctly predicted hits + correctly predicted no-hits) / (total hits + total no-hits)

$$OR = [(1 - FN)(%H) + (1 - FP)(%NH)] / [(1 - FN)(%H) + (1 - FP)(%NH) + FP(%NH) + FN(%H)]$$

Summary of Reliability Results for Low and High Screens Based on EPA 2009

EPA	Samples	Hits	No-Hits	%False Negatives	%False Positives	Hit Reliability	NoHit Reliability	PredHit Reliability
postBERA pooled lo	293	108	185	19.4	53.0	80.6	47.0	47.0
postBERA pooled hi	293	65	228	20.0	35.1	80.0	64.9	39.4
CH G lo	293	52	241	19.2	21.2	80.8	78.8	45.2
CH G hi	293	42	251	19.0	13.9	81.0	86.1	49.3
CH S lo	293	44	249	18.2	26.5	81.8	73.5	35.3
CH S hi	293	32	261	18.8	12.3	81.3	87.7	44.8
HY G lo	293	75	218	20.0	54.1	80.0	45.9	33.7
HY G hi	293	39	254	17.9	33.9	82.1	66.1	27.1
HY S lo	293	21	272	19.0	4.4	81.0	95.6	58.6
HY S hi	293	19	274	15.8	4.7	84.2	95.3	55.2

PredNoHit	Overall Reliability
80.6	59.4
91.9	68.3
95.0	79.2
96.4	85.3
95.8	74.7
97.4	87.0
87.0	54.6
96.0	68.3
98.5	94.5
98.9	94.5